

Nanotechnologies / Materials

Smart device, Phototransistor, Sensing materials



Development of colorless organic semiconducting materials response to NIR light

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Researchmap https://researchmap.jp/Soichi_Yokoyama?lang=en Researchmap https://researchmap.jp/read0105668?lang=en



Abstract

The development of colorless and transparent π -conjugated molecules with near-infrared (NIR) light-selective absorption is expected for the applications in organic semiconducting materials such as NIR imaging or sensing materials and colorless/transparent organic solar cells. However, the development of the colorless NIR dye is still behind because the guidelines of the molecular design are not yet established. In this study, we propose a molecular design strategy based on tuning molecular orbital symmetries to accomplish colorless and transparent organic semiconducting materials with selective near-infrared light absorption. Based on the Laporte rule, a selection rule for electronic transitions, the building units were carefully determined to permit only electronic transitions related to NIR absorption. The designed molecule FNTz-Py showed a colorless and transparent feature in both solution and thin film with selective NIR absorption properties. Furthermore, we successfully demonstrated that the transistor devices based on FNTz-Py selectively responded to near-infrared light.

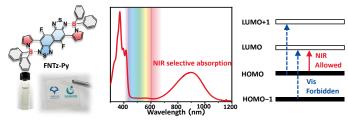
Background & Results

Organic semiconducting materials that respond to NIR light, which is an invisible component of sunlight, are expected to the development of novel applications such as imaging or sensing materials for near-infrared light and colorless/transparent organic solar cells. However, the development of organic semiconductor materials with "near-infrared light-selective absorption properties" have been limited due to the lack of established guideline for molecular design. In this study, we aimed to establish a molecular design to develop the organic semiconducting materials that exhibit NIR-selective absorption.

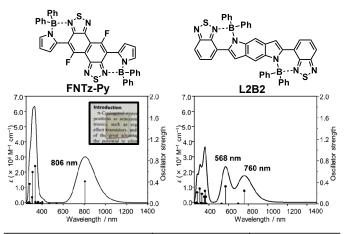
To design materials with selective NIR light absorption, it is essential to 1) narrow the molecular bandgap sufficiently to reach NIR regime and 2) allow electronic transitions in the NIR region while electronic transitions in the visible region should be forbidden. This selection rule for electronic transitions can be achieved by tuning molecular symmetries according to the Laporte rule. Based on this theory, we designed and synthesized a donor-acceptor-donor type molecule FNTz-Py. This molecule showed selective NIR absorption, providing a colorless and transparent solution and film. Theoretical calculations indicated that electronic transition in the NIR regime is allowed while those in the visible regime are forbidden. In addition, transistor devices based on FNTz-B exhibited a selective response to near-infrared light.

Significance of the research and Future perspective

The energy from NIR light is rarely utilized in silicon and perovskite solar cells while the energy is accounted for up to 30% of sunlight. The development of colorless and transparent organic solar cells, which can convert near-infrared light into electrical energy, is expected by utilizing our proposed molecular design.

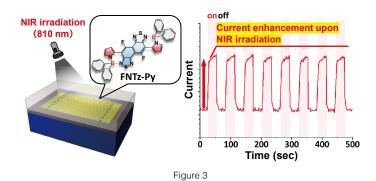






		FNTz-Py	L2B2
Excited State	Electronic transitions	MO symmetries and Selection rule	MO symmetries
S ₁	HOMO→LUMO	$u \rightarrow g \ O$ Allowed	$\textbf{g} \rightarrow \textbf{u} ~ \textbf{O} ~ \textbf{Allowed}$
S ₂	HOMO→LUMO+1	$\mathbf{u} \rightarrow \mathbf{u} \times Forbidden$	$\mathbf{g} \rightarrow \mathbf{g} \times Forbidden$
S₃	HOMO-1→LUMO	$\mathbf{g} \rightarrow \mathbf{g} \mathbf{X}$ Forbidden	$\textbf{g} \rightarrow \textbf{u} ~ \textbf{O} ~ \textbf{Allowed}$

Figure 2



Patent PCT/JP2025/005511 Yokoyama, Soichi; le, Yutaka. Fluorinated dihydropentalene-1,4-dione: a strong electron-accepting unit with organic semiconductor characteristics. Chem. For J. 2022/03873. doi: 10.1002/chem.2022/03873 Yokoyama, Soichi; le, Yutaka et al. Colorless near-infrared absorbing dyes based on B-N fused donor-acceptor-donor π -conjugated molecules for organic phototransistors. Adv. Sci. 2024, 11, 2405656. doi: 10.1002/advs.202405656 https://www.sanken.osaka-u.ac.jp/labs/omm/

Keyword NIR-absorbing dye, organic semiconducting materials, organic functional materials